Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Methyl 2-selenocyanatobenzoate

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Received 18 October 2002
Accepted 21 October 2002
Online 25 October 2002

The title compound, $C_9H_7NO_2Se$, displays an intramolecular Se···O contact of 2.5614 (15) Å and an intermolecular Se···N contact of 3.271 (2) Å. The molecule is approximately planar, the substituents being rotated by *ca* 5° out of the ring plane.

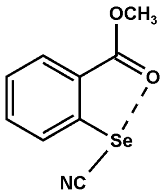
Key indicators

Single-crystal X-ray study
T = 133 K
Mean σ(C–C) = 0.002 Å
R factor = 0.018
wR factor = 0.045
Data-to-parameter ratio = 21.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Selenocyanates are commonly used as intermediates in the synthesis of diorganoselenates (Toshimitsu & Uemura, 1987). Recently, areneselenocyanates, such as benzylselenocyanate and 1,2-, 1,3- and 1,4-phenylenebis(methylselenocyanate), have been used as antitumour drugs (Shimida *et al.*, 1997; Mugesh *et al.*, 2001). Organoselenium compounds exhibiting intramolecular Se···O interactions are particularly interesting, since these interactions are expected to modulate the biological activity of the selenium compounds (Burling & Goldstein, 1992; Goldstein *et al.*, 1994; Wirth, 1998). The structure of the title compound, (I), was determined in this context.



(I)

The molecule (Fig. 1) shows the expected intramolecular Se···O interaction, with a distance of 2.5614 (15) Å, significantly shorter than the sum of the van der Waals radii (3.42 Å). A rather longer contact was observed in the related compound, phenacyl selenocyanate [2.722 (2) Å; Maartmann-Moe *et al.*, 1986]. The title compound may thus be considered as a three-coordinate selenium complex, with the Se···O interaction *trans* [angle C9—Se—O1 170.34 (7)°] to the cyano group. The C—Se—C bond angle of 94.68 (7)° is similar to those in other selenocyanates, *e.g.* 96.0° in benzylselenocyanate, 94.0° in 4-nitrobenzyl selenocyanate (Maartmann-Moe *et al.*, 1984), 95.1° in phenacyl selenocyanate (Maartmann-Moe *et al.*, 1986), 94.4° in 1,4-diselenocyanatobenzene (McDonald & Pettit, 1970) and 95.9 (3)° in 1,2-phenylenebis(methylselenocyanate) (McWhinnie *et al.*, 1998). The Se—CN bond length of 1.8720 (19) Å in the present structure is slightly longer than those observed previously, which range from 1.775 (McWhinnie *et al.*, 1998) to 1.845 Å (Maartmann-Moe *et al.*, 1986).

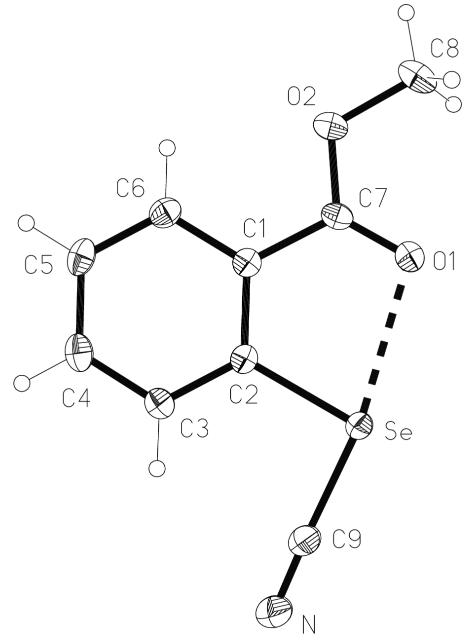


Figure 1
The molecule of the title compound in the crystal. Ellipsoids are drawn at the 50% probability level. H-atom radii are arbitrary. The Se···O contact is indicated by a broken bond.

The molecule is essentially planar (mean deviation of all non-H atoms 0.042 Å). The substituents are rotated out of the ring plane by *ca* 5° (Table 1).

The molecules are linked, *via* the 2_1 screw operator, by an Se···N contact of 3.271 (2) Å (Fig. 2).

Experimental

Methyl 2-selenocyanobenzoate was prepared as described by Iwaoka & Tomoda (1992). Single crystals were grown from a concentrated solution in diethyl ether by slow evaporation.

Crystal data

$C_9H_7NO_2Se$
$M_r = 240.12$
Orthorhombic, $Pna2_1$
$a = 7.4707$ (3) Å
$b = 16.3734$ (7) Å
$c = 7.2188$ (3) Å
$V = 883.01$ (6) Å^3
$Z = 4$
$D_x = 1.806$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 4106 reflections
$\theta = 5$–$12.5°$
$\mu = 4.21$ mm^{-1}
$T = 133$ (2) K
Prism (cut), pale yellow
0.39 × 0.21 × 0.14 mm

Data collection

Bruker SMART 1000 CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{\min} = 0.630$, $T_{\max} = 0.895$
11007 measured reflections

2516 independent reflections
2387 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\max} = 30.0°$
$h = -9 \rightarrow 10$
$k = -23 \rightarrow 23$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.018$
$wR(F^2) = 0.045$
$S = 1.01$
2516 reflections
119 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.62$ e Å^{-3}
$\Delta\rho_{\min} = -0.33$ e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter = 0.030 (7)

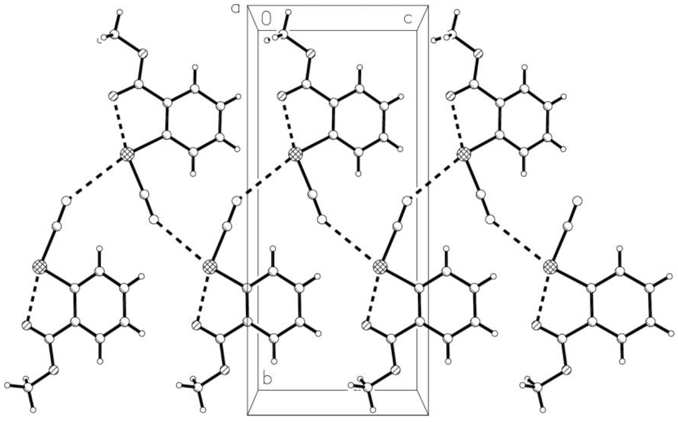


Figure 2
Packing diagram of the title compound, viewed down the *a* axis. The Se···O and Se···N contacts are indicated by broken bonds.

Table 1
Selected geometric parameters (Å, °).

Se—C9	1.8735 (19)	Se—O1	2.5608 (15)
Se—C2	1.9365 (15)		
C9—Se—C2	94.72 (7)	C2—Se—O1	76.66 (5)
C9—Se—O1	170.34 (7)	C7—O1—Se	102.97 (11)
C9—Se—C2—C3	6.50 (14)	C2—C1—C7—O1	−5.1 (2)

The structure could not be solved by direct methods in either of the space groups consistent with the systematic absences (*Pnma* or $Pna2_1$). The Se-atom position was therefore determined *via* the Patterson function in $Pna2_1$ and the structure gradually expanded by successive difference syntheses; the double image generated by the presence of one heavy atom proved troublesome throughout. The absolute structure (polarity) was determined on the basis of 1217 Friedel pairs. Methyl H atoms were located in difference syntheses, idealized (C—H 0.98 Å and H—C—H 109.5°) and refined on the basis of rigid groups allowed to rotate but not tip. Other H atoms were included using a riding model with fixed C—H bond lengths of 0.95 Å; $U_{\rm iso}$(H) values were fixed at $1.2U_{\rm eq}$ of the parent atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL*97.

Financial support from the Fonds der Chemischen Industrie is gratefully acknowledged. We thank Mr. A. Weinkauf for technical assistance.

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